

Test possibility of using near and mid infrared spectroscopic techniques to predict mycotoxin concentrations in barley and wheat

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Wheat and barley are ranked among the most important crops in western Canada. However, they have been suffering from mycotoxins contamination for a long time. The application of traditional methods is time consuming and requires a high level of experience and expertise. There is an urgent need for a fast and simple screening method. A total of 80 wheat and 42 barley samples were collected and detected for 6 major ergot alkaloids as well as other 12 common mycotoxins concentration by liquid chromatography-tandem mass spectrometry method. The near-infrared spectra (NIR; 680-2500 nm) and mid-infrared spectra (MIR; 4000-700 cm^{-1}) of all samples were collected with the NIR and FT/IR spectrometers. All spectra were averaged from three repeat NIR or FT/IR measurements, each recorded from a new sub-sample. The final spectra data were imported into the Unscrambler X, v10.3 (CAMO, Oslo, Norway). Some preliminary descriptive analyses were performed by both graphic tools and numerical results. To remove the spectral baseline shift, noise, and light scatter effects, nine preprocessing methods were applied, including baseline offset, standard normal variate (SNV), detrending, SNV + detrending, multiplicative scatter correction, first derivative, second derivative, first derivative + SNV, and second derivative + SNV. The possibility of whether we can develop a fast screening method for wheat and barley mycotoxins detecting by NIR and MIR is expected to be revealed when the calibration and validation procedure is completed.